



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

## ICAMS Special Seminar

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Wednesday June 26, 11:15 a.m. ICAMS Seminar room 0.07

### Application of the phase-field method to modeling microstructure evolution in Li-ion batteries

Phase-field method has been applied to modeling mesoscale microstructure evolution in many different processes including phase transformations and microstructure coarsening. This presentation will give a brief introduction to the phase-field method and discuss its applications to microstructural processes during Li-plating and Li-insertion into and extraction from electrodes in Li-ion batteries. The focus will be on  $\text{Li}_x\text{FePO}_4$ , one of the most-studied cathode materials in Li-ion batteries. The thermodynamics of the  $\text{FePO}_4$ - $\text{LiFePO}_4$  two-phase system and the effect of coherent stress on the miscibility gap and two-phase morphology will be discussed. A three-dimensional phase field model for modeling the morphological evolution during the intercalation/extraction of Li-ions into a host electrode will be described. It incorporates the effects of anisotropic diffusional mobility of Li-ions in the electrode host lattice, flux of Li-ions across the electrode/electrolyte interface, and coherency strains arising from the lattice parameter mismatch between the lithiated and unlithiated phases. Implementation of spectral methods to solving the systems of equations under non-periodic boundary conditions will be presented. The microstructural features obtained from the simulations are compared with available experimental observations.

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